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Title: Modeling Marangoni Effect in Liquid-Liquid Microfluidic Systems

Author(s): Root, Alison Hayley

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Modeling Marangoni Effect in Liquid-Liquid Microfluidic Systems

Alison Root

Mentors: Garrison Stevens (MET-1) and Scott Ouellette (W-13)

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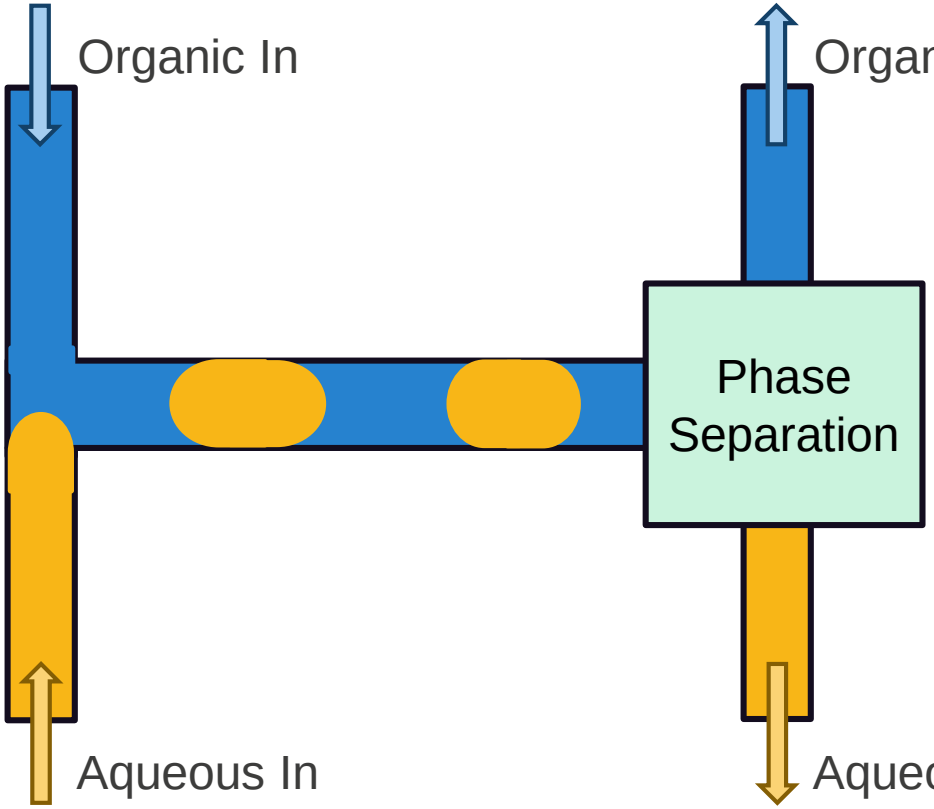
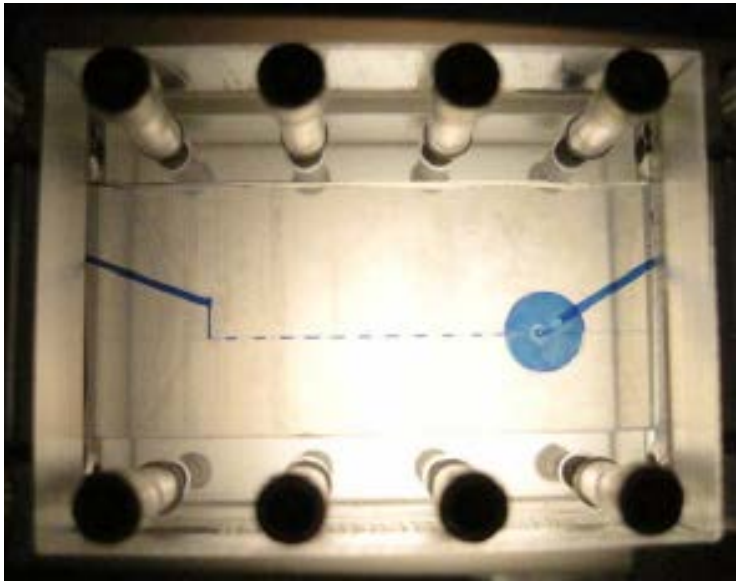
Microfluidics presents opportunities for high mass transfer rates between fluids within a small device

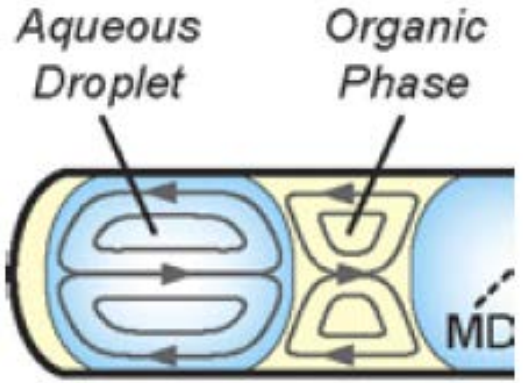




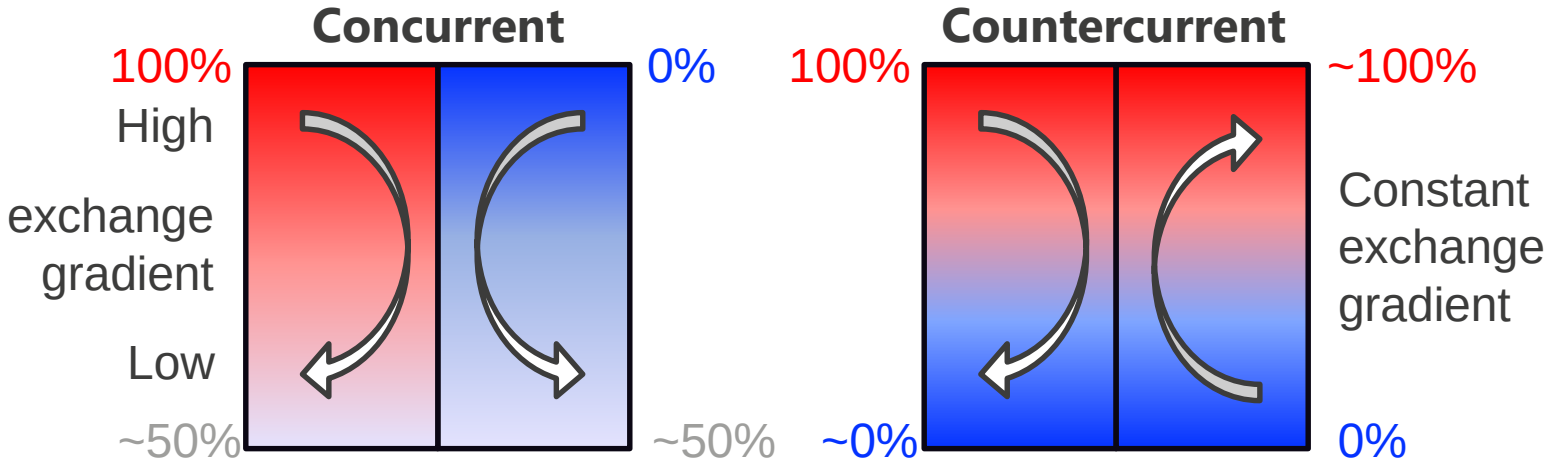
$$CH_3COOH + KOH \rightarrow CH_3COOK + H_2O$$

Benefits of droplets in a two-phase flow channel

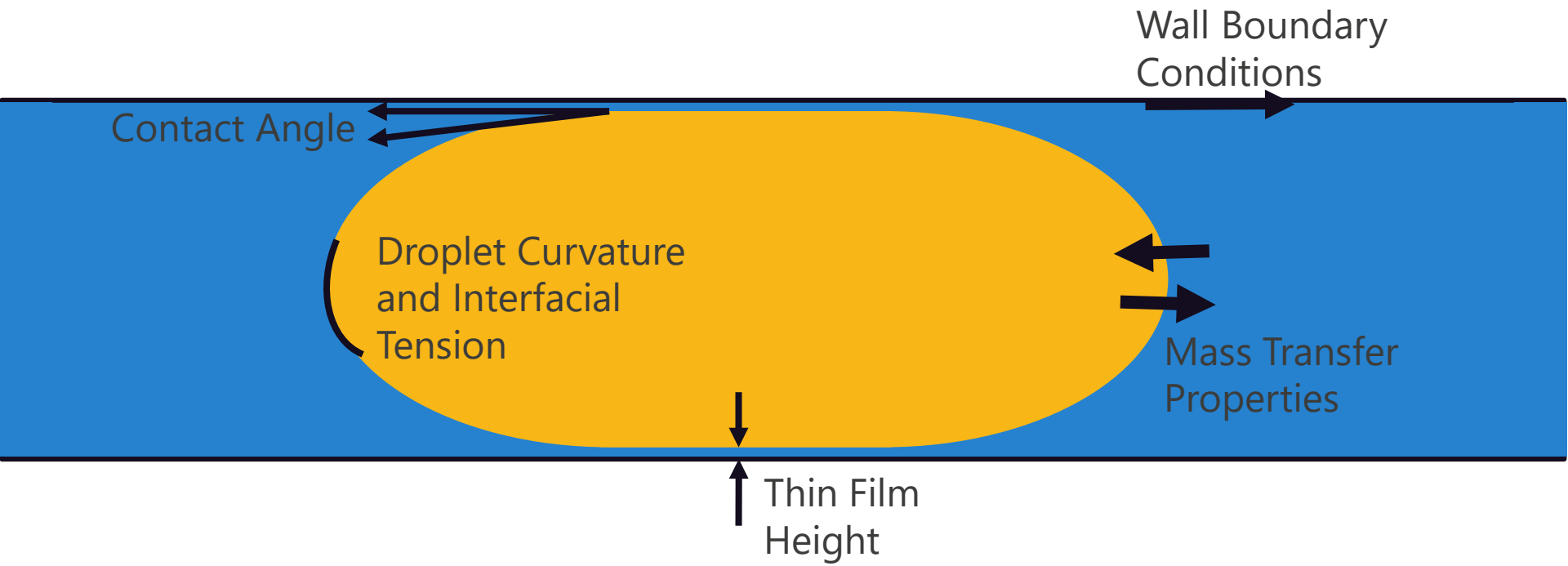
- **Droplets are beneficial for mass transfer due to the maximal surface area between the two fluids and the development of countercurrent flow**



Flow inside individual "slugs"
Nichols, et al., J. Am. Chem. Soc., 133, (2011), 15721-15729



Uncertain parameters and measurements of interest in the model



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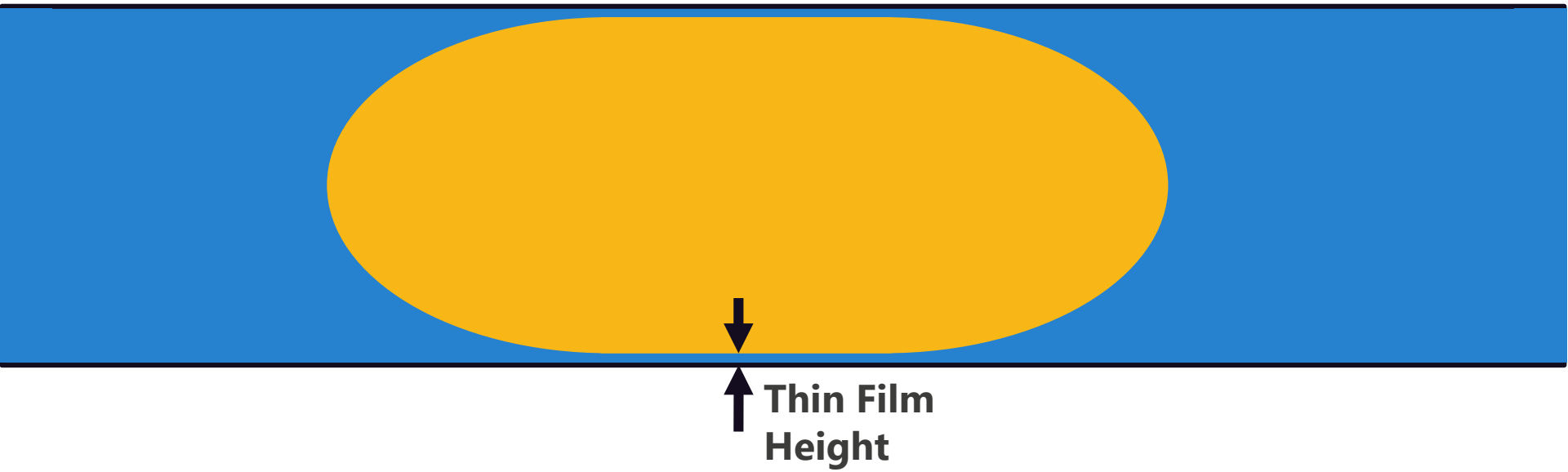
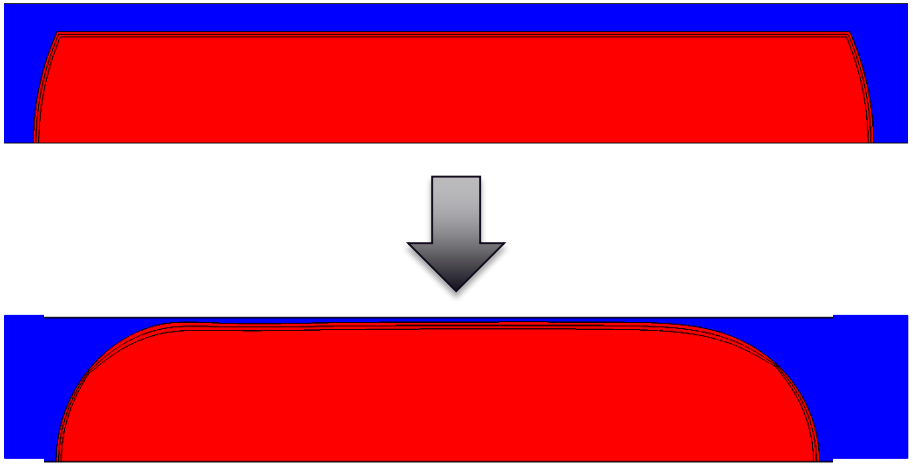
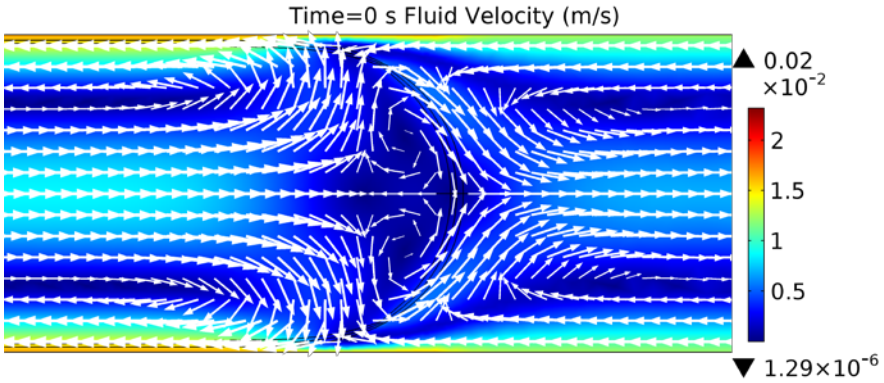


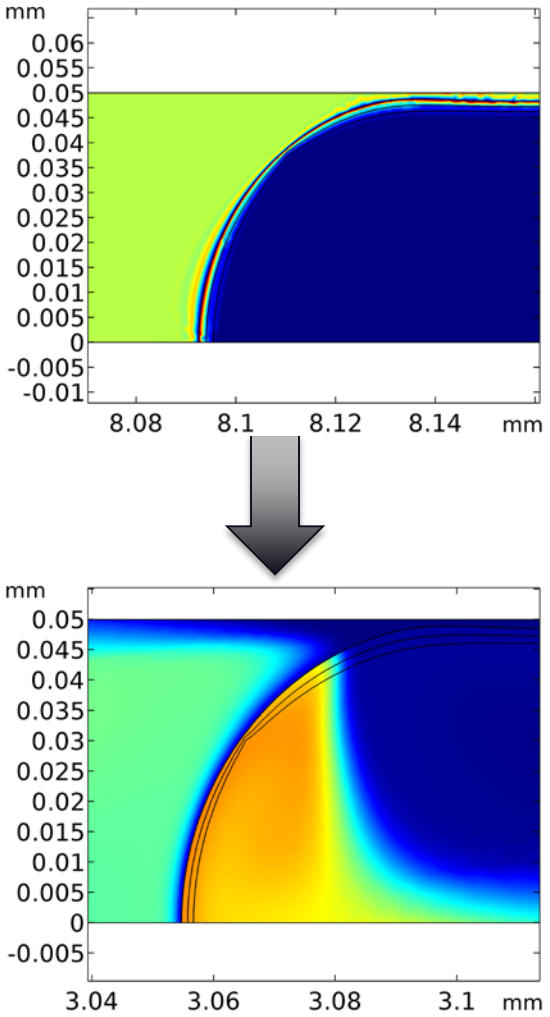
The model consists of two steps, one to establish fluid flow and droplet shape and one for mass transfer

Moving Mesh

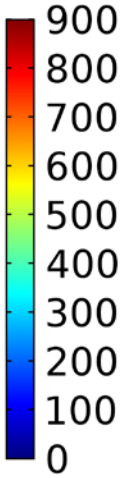




Mass Transfer

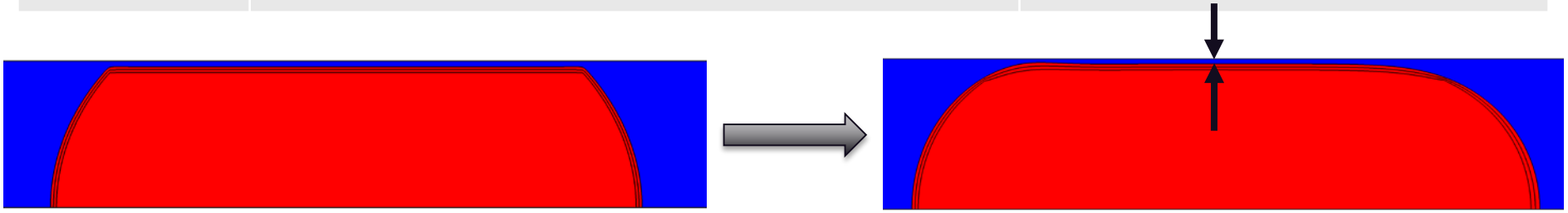


Acetic Acid Concentration (mol/m^3)

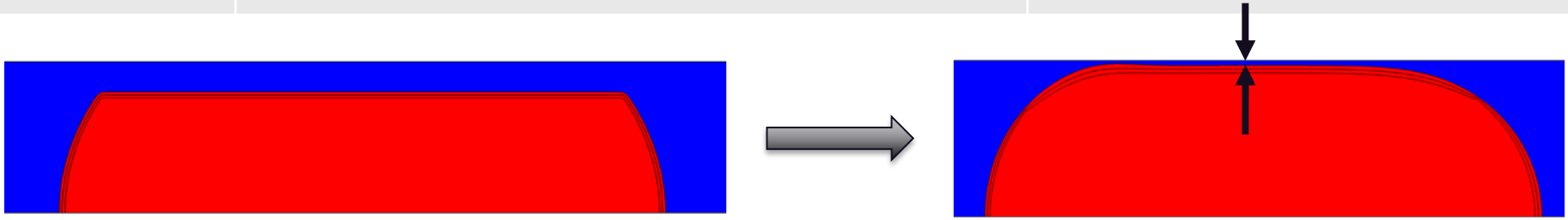


Converged droplet shape for initial length of 0.2 mm

Time (s)	Thin Film Height at Center (mm)	Droplet Length (mm)
0	0.001	0.202
0.5	0.01341	0.2084

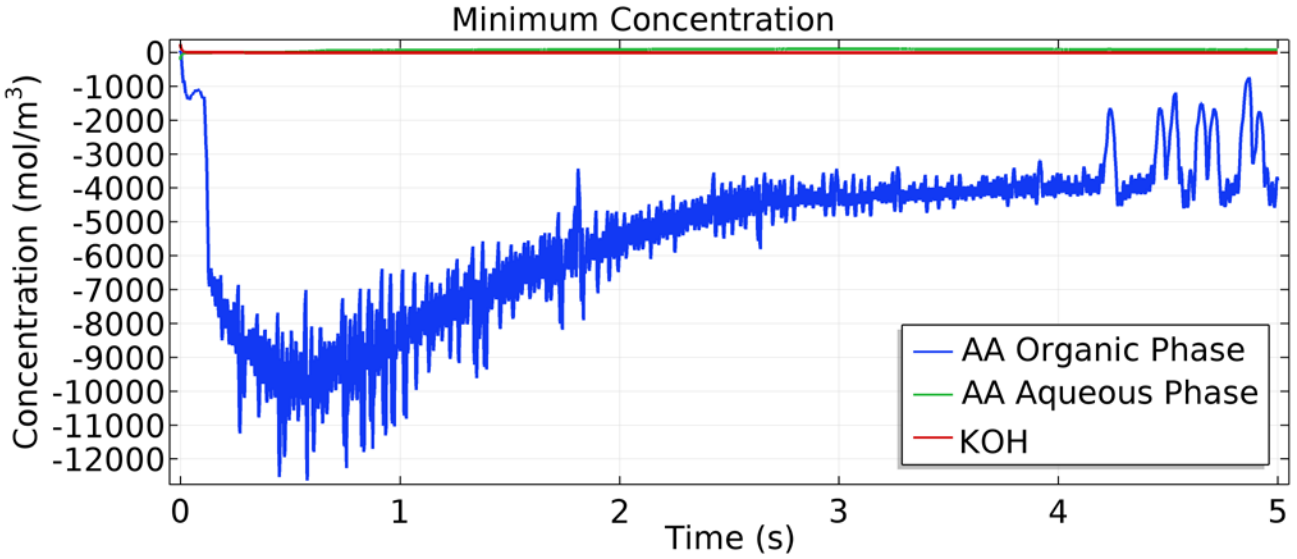


Time (s)	Thin Film Height at Center (mm)	Droplet Length (mm)
0	0.010	0.202
0.5	0.01505	0.1800

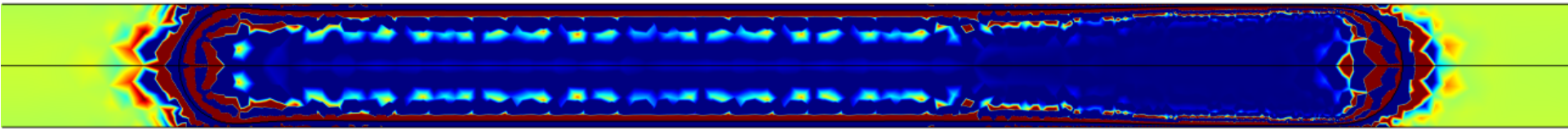


Numerical errors are common in convection and diffusion problems with sharp boundaries

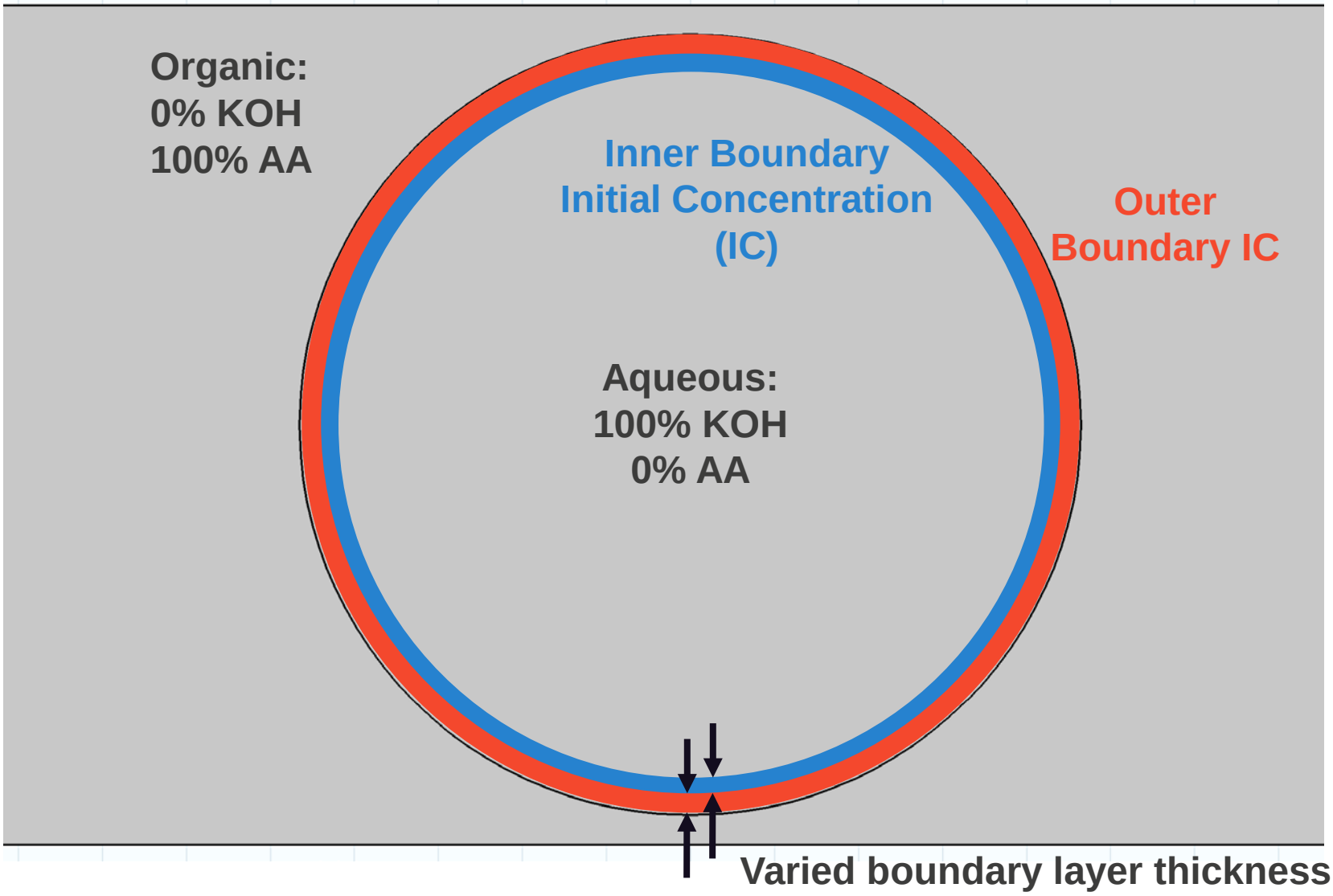
- **Negative concentrations**



- **System mass not conserved**
- **Strange numerical behavior**

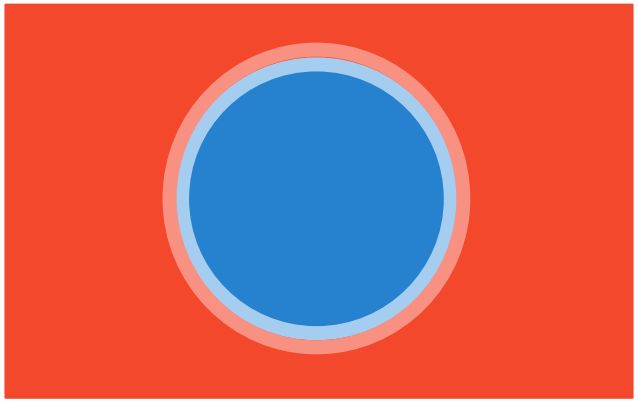


A toy model was investigated to look for ways of reducing numerical errors in the mass transfer



Several types of initial concentration conditions were tested with this model

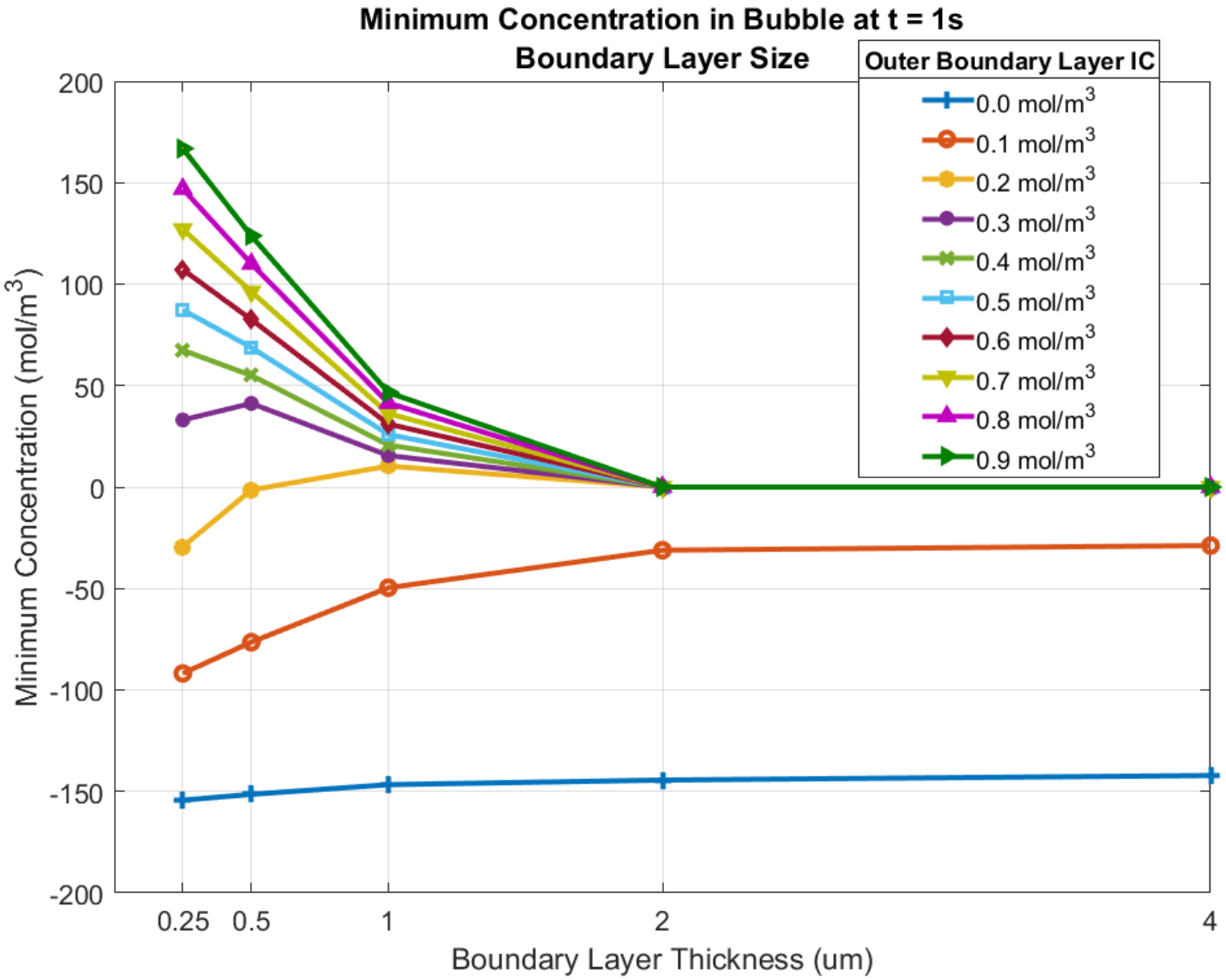
Initial concentrations in original model (no boundary layers)



Initial concentrations with boundary layers

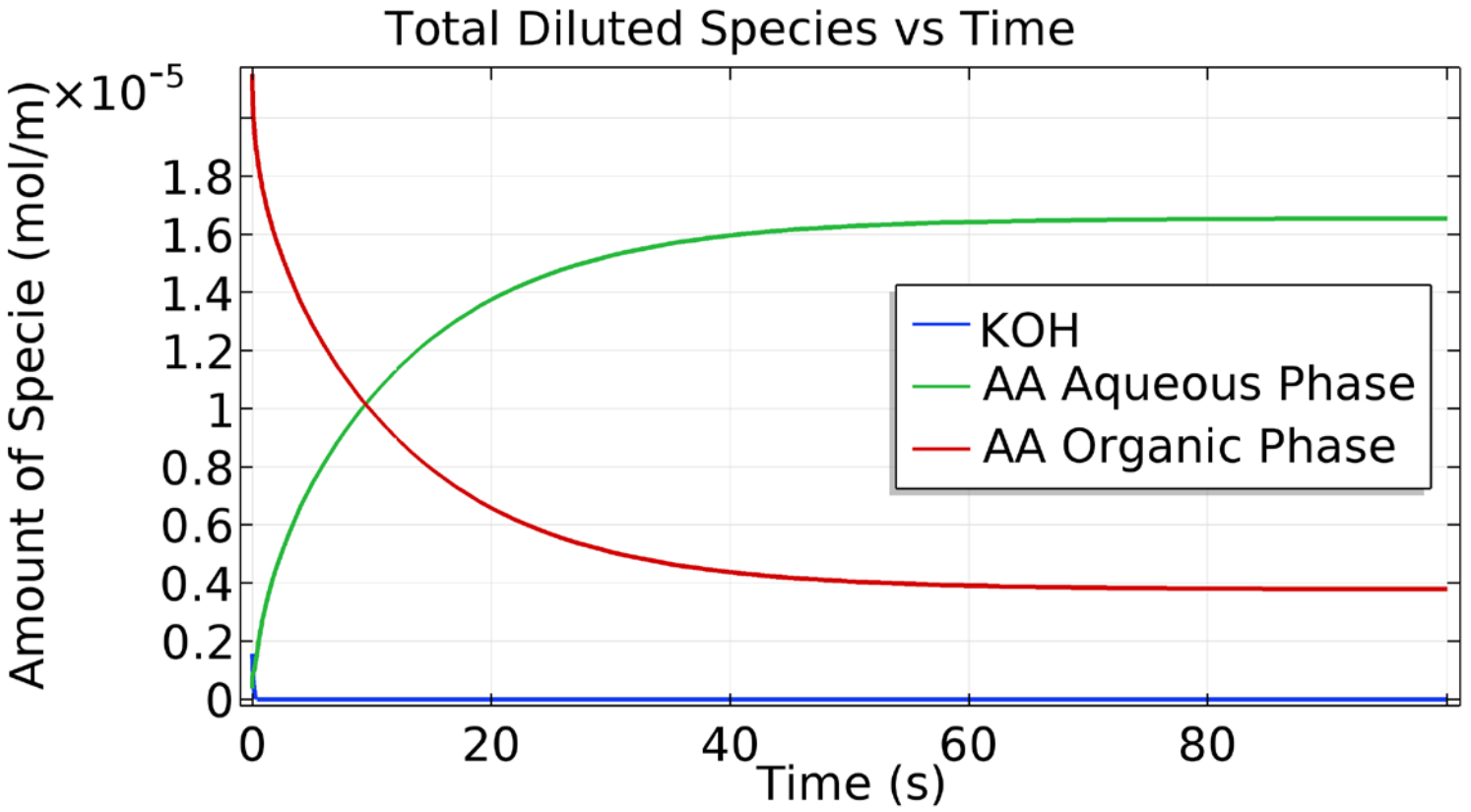
Initial concentrations with smoothing in boundary layers

Parametric studies of boundary layer thickness and concentrations in the toy model helped find ways to reduce numerical errors in the mass transfer

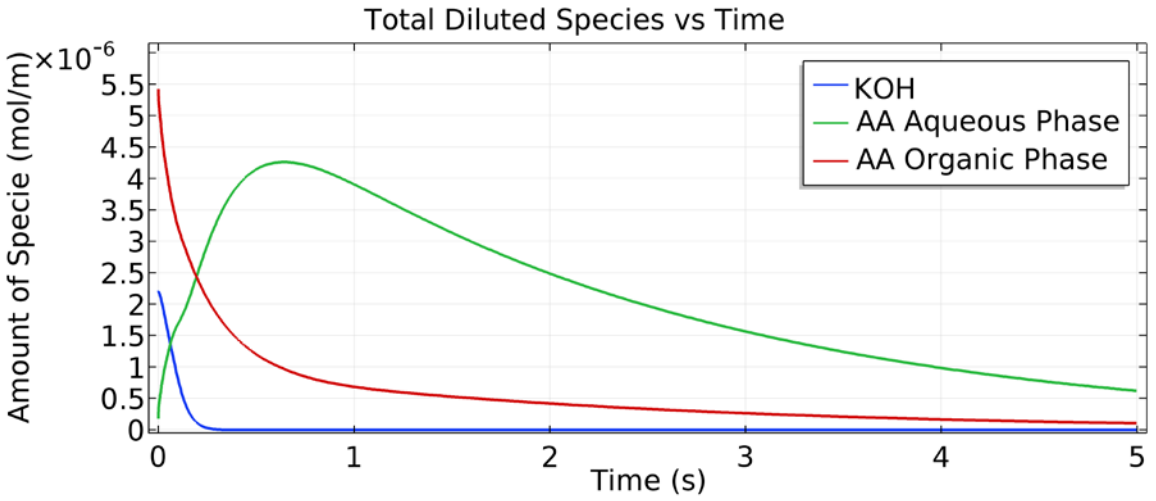


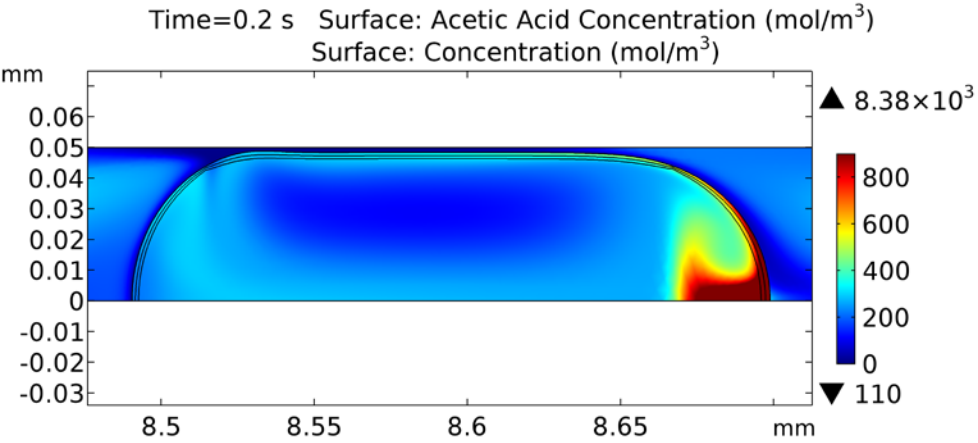
The behavior seen in the toy model using some combinations of parameters is what is expected from mass transfer

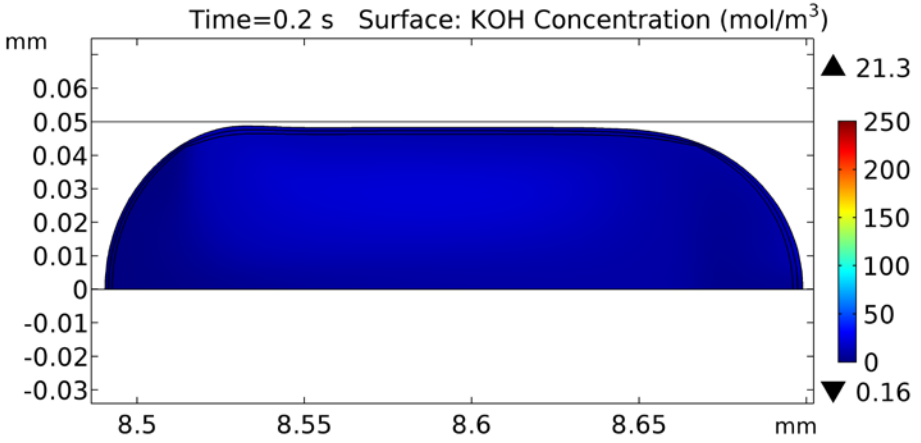
- **Total acetic acid is constant after KOH has reacted away**
- **Parameters for this behavior:**
  - Thicker boundary layers (at least 1 μm)
  - Outer boundary layer concentration at least 20% of concentration inside droplet



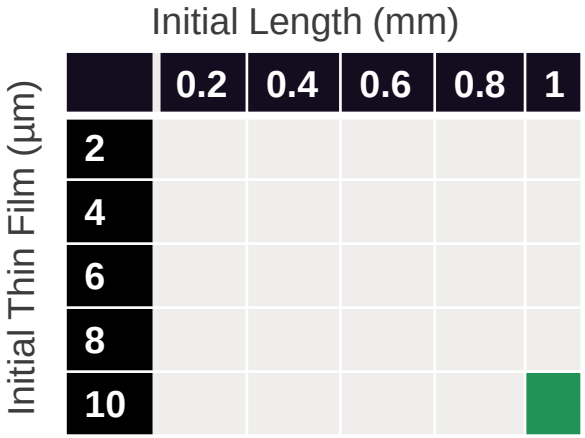
Using parameters that worked in the toy model gives better mass transfer results in the full-physics model

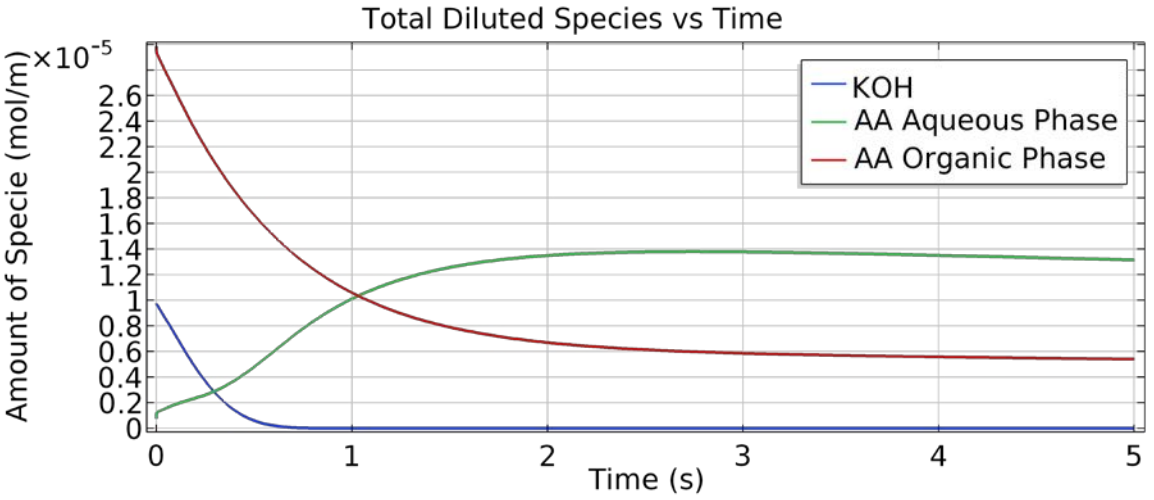


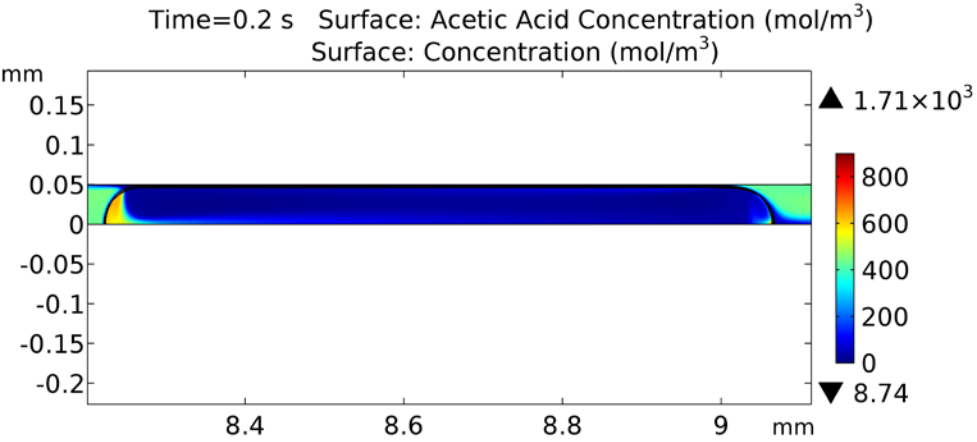


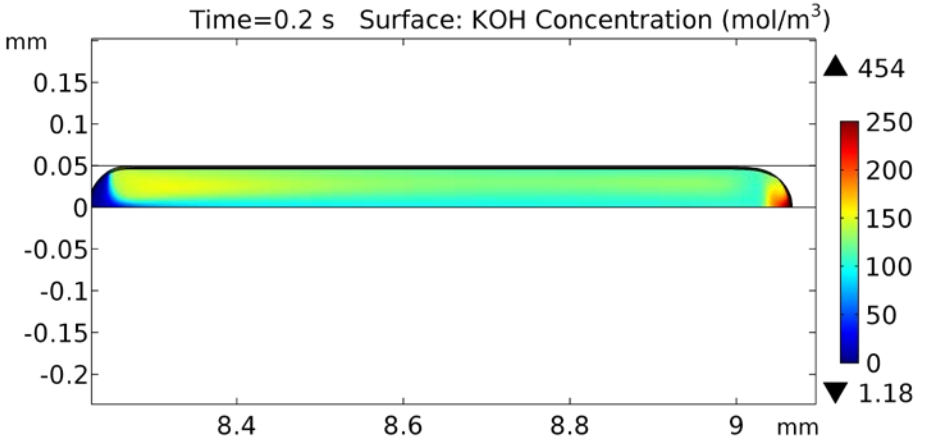


Again, changing initial thin film height but keeping length constant has a minimal effect on mass transfer

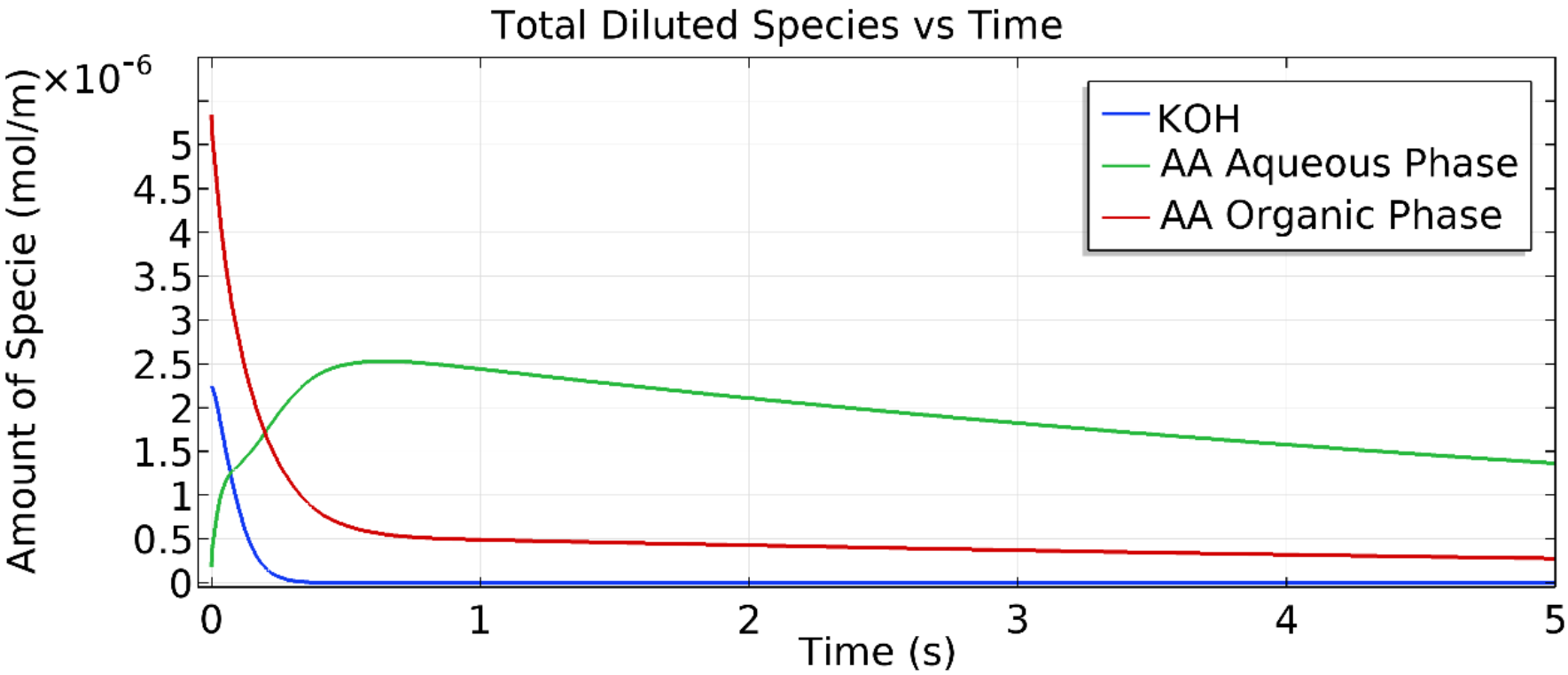






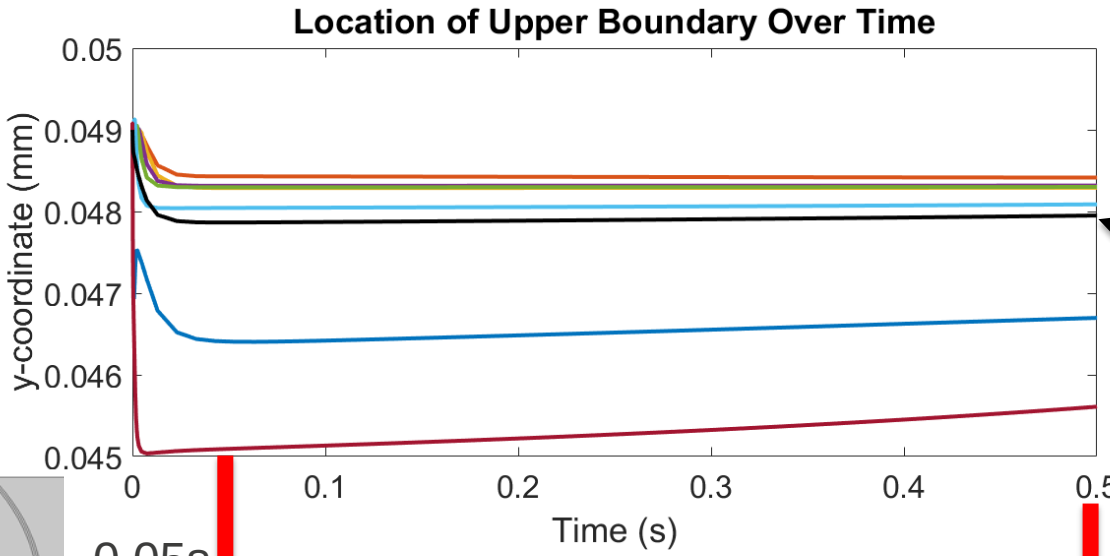


This version of the mass transfer step is much better than before, but there are still problems



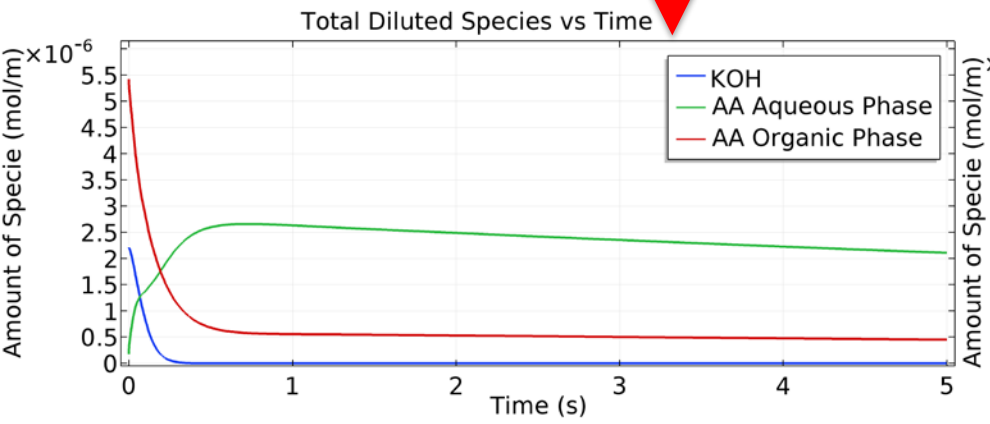
- **Conservation of mass is still not ensured**
- **Alleviated with more stable bubble, but still not perfect**
  - Can bubble not stabilize fully?
  - Is there some other problem?

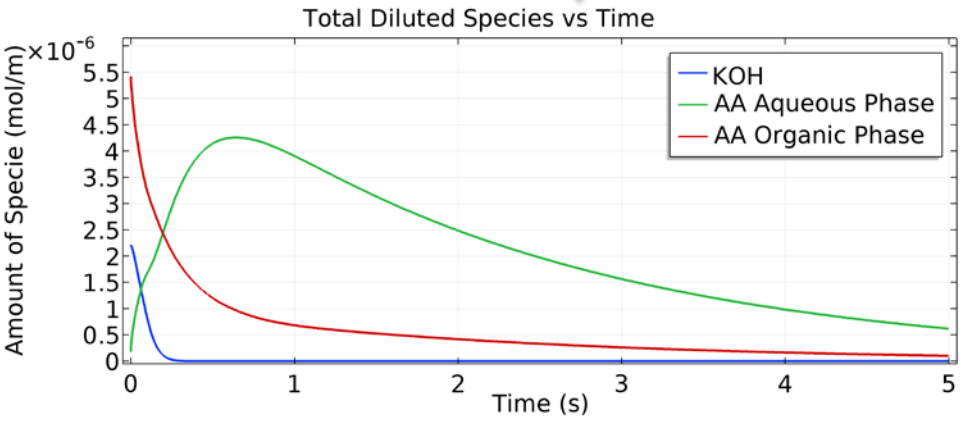
When the droplet is in a more stable state from the moving mesh step, the mass transfer step is better



Average location of entire boundary

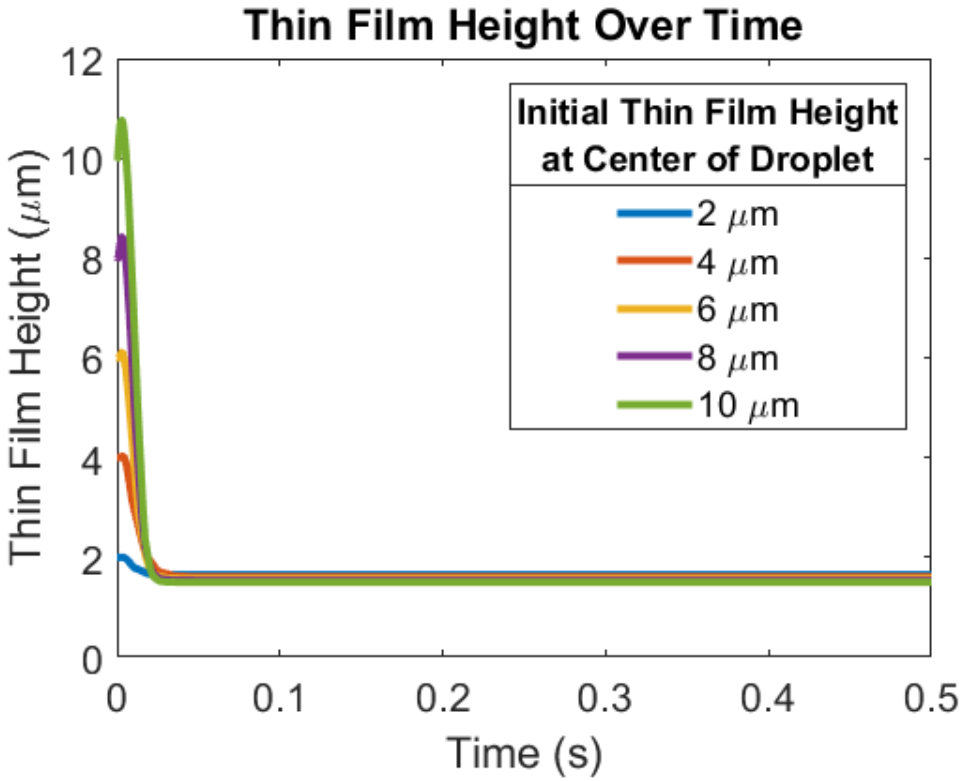
0.05s





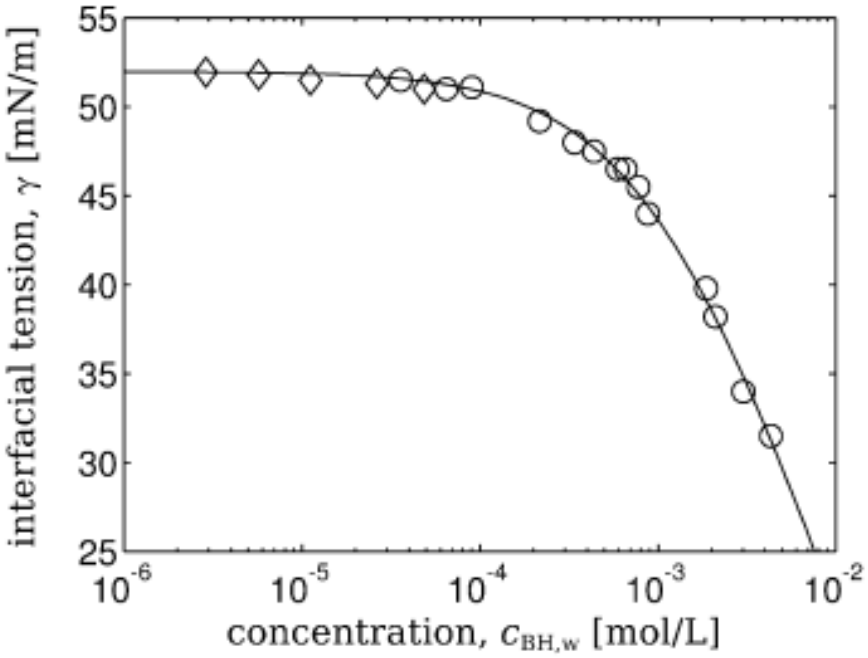
Conclusions

- **Developed a droplet model that takes thin film height into account.**
- **Studied numerical errors in mass transfer models.**
- **Droplet tends to converge to a similar height at the same flow parameters regardless of initial size.**
  - Can predict thin film height based on flow parameters



Future work

- **Fix problem with acetic acid loss**
- **Combined model**
  - One model that does moving mesh and mass transfer simultaneously
  - Mass transfer affects interfacial tension, but does interfacial tension affect droplet shape?



Fricke and Sundmacher. *Langmuir*. **2012**. *28*, 6803-6815.

Thank you!
Questions?

ahroot@princeton.edu